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Novel 2D triple-resonance NMR experiments for sequential resonance assignments of proteins.

Ding K, Gronenborn AM.
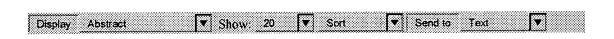
Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, Maryland 20892, USA.

We present 2D versions of the popular triple resonance HN(CO) CACB, HN(COCA)CACB, HN(CO)CAHA, and HN(COCA) CAHA experiments, commonly used for sequential resonance assignments of proteins. These experiments provide information about correlations between amino proton and nitrogen chemical shifts and the alpha- and beta-carbon and alpha-proton chemical shifts within and between amino acid residues. Using these 2D spectra, sequential resonance assignments of H(N), N, C(alpha), C(beta), and H(alpha) nuclei are easily achieved. The resolution of these spectra is identical to the well-resolved 2D (15)N-(1)H HSQC and H(NCO)CA spectra, with slightly reduced sensitivity compared to their 3D and 4D versions. These types of spectra are ideally suited for exploitation in automated assignment procedures and thereby constitute a fast and efficient means for NMR structural determination of small and medium-sized proteins in solution in structural genomics programs.

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